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Topological Effects in 1-Pentagon Carbon Nanocones: Migrating Faces and Magic sizes

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Abstract

Changes in topology descriptors of one-pentagon carbon nanocones are investigated using both, direct F and dual graph F^D representations. *Topological compactness* and *topological roundness* - described by Wiener index W and topological efficiency ρ index respectively - dominate the growth of such a structure. Various chemical implications are forecasted on the basis of our purely topological model.

Key words: carbon nanocones, topological compactness, topological roundness
MSC2000: AMS Codes (none)

1. Introduction

Variations of the topological features of carbon nanocones with one pentagon at the apex (1-P NANOCONE) are investigated using both direct F and dual graph F^D representations. In this work we derived the asymptotic values for two important topological indices, the Wiener number W and the topological efficiency ρ index, improving previous numerical studies [1]. The two invariants are distance-based topological descriptors that, by taking into account the long-range structure of the graphs, describe important structural characteristics of the underlying nano-system, *i.e.* its *topological compactness* (W) and *topological roundness* (ρ).

Both indices drive the growth of such a structure when successive circles f of carbon atoms are added to it ($f \geq 0,1,2\ldots$, $f=0$ corresponding to the isolated pentagon case). When the 1-P NANOCONE is represented in the direct space (the N nodes of the graph correspond to the N carbon atoms of the chemical structure), the graph invariants follow the asymptotic curves reported in the box below.

F is made by 1 pivotal pentagon P surrounded by f concentric belts of hexagons $f = 0, 1, 2, 3, \ldots$.

Total number of hexagons is:
$n_6 = \frac{5}{2}(f^2 + f)$

Total number of faces $n_T = n_5 + n_6 = n_6 + 1$

for $f=0$ then $n_T = n_5 = 1$

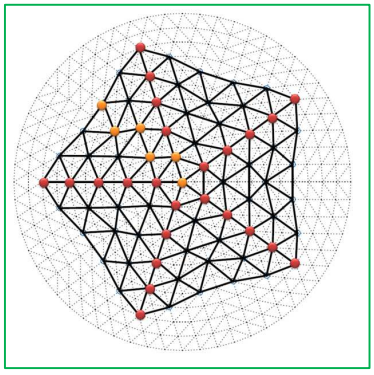
The number of nodes (carbon atoms) N obeys to the rule:
$N = 5 + 5(f^2 + 2f)$

Wiener index goes like:
$W(f) = (124f^5 + 620f^4 + 1205f^3 + 1135f^2 + 516f + 90)/6$

Other 1-P NANOCONE invariants have been derived in F and F^D.

2. Some Results

Present topological modelling is rich of original results on the chemical features of the nanocones, that are really very hard to achieve just by employing ab-initio investigations.



First of all, our topo-simulations show that the position of the most stable hexagonal face varies as a function of the nanocone size f, influencing in such a

way the stability of the whole structure (see the yellow path in the figure above). This migration follows a sequence of peculiar "jumps" in correspondence of specific *f* values.

Moreover, for certain numbers of hexagons (*magic sizes*), the conic cage results topologically more stable than graphenic fragments having similar number of atoms. Topological features make then 1-P NANOCONE suitable for generating fullerene-like structures whose presence in carbon black graphene sheets or in activated carbon has many experimental implications. The importance of fullerene-like structures also involves the interstellar carbon dust, playing in such a way a crucial role in catalyzing the formation of molecular hydrogen and other low-temperature chemical reactions.

3. References

[1] F. CATALDO, O. ORI AND S. IGLESIAS-GROTH, *Topological lattice descriptors of graphene sheets with fullerene-like nanostructures,* Mol. Sim., **36** (2010), 341.